LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005399.D
Acq On : 23 Apr 2021 18:14
Operator : CG/JU
Sample : M2149-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-40-9.5-10.0

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.781	283	288	293	rBV	20217	28098	1.39%	0.311%
2	5.234	359	365	376	rBV	588705	826391	40.87%	9.133%
3	6.822	627	635	649	rBV	578079	937195	46.35%	10.358%
4	7.634	766	773	781	rBV	100436	157878	7.81%	1.745%
5	8.799	963	971	983	rBV	377115	625425	30.93%	6.912%
6	10.422	1240	1247	1256	rBV	105406	179925	8.90%	1.989%
7	12.910	1663	1670	1678	rBV	734745	1059065	52.38%	11.705%
8	13.769	1811	1816	1823	rBV2	15992	25810	1.28%	0.285%
9	14.299	1900	1906	1915	rBV	146655	220981	10.93%	2.442%
10	15.804	2156	2162	2173	rBV	687136	970994	48.02%	10.731%
11	17.069	2369	2377	2387	rBV	198372	287643	14.23%	3.179%
12	17.969	2525	2530	2539	rBV	41831	70325	3.48%	0.777%
13	19.216	2738	2742	2753	rBV3	21721	33511	1.66%	0.370%
14	19.475	2776	2786	2793	rBV3	27335	110675	5.47%	1.223%
15	19.651	2810	2816	2828	rVB	1739024	2022081	100.00%	22.348%
16	20.851	3016	3020	3022	rBV3	22678	36045	1.78%	0.398%
17	20.886	3022	3026	3034	rVV2	189724	307214	15.19%	3.395%
18	20.957	3035	3038	3044	rVB	62192	81185	4.01%	0.897%
19	21.175	3070	3075	3081	rBV	368675	433631	21.44%	4.792%
20	21.775	3173	3177	3186	rVB2	97361	181548	8.98%	2.006%
21	23.433	3453	3459	3468	rVB	242875	452499	22.38%	5.001%

Sum of corrected areas: 9048119

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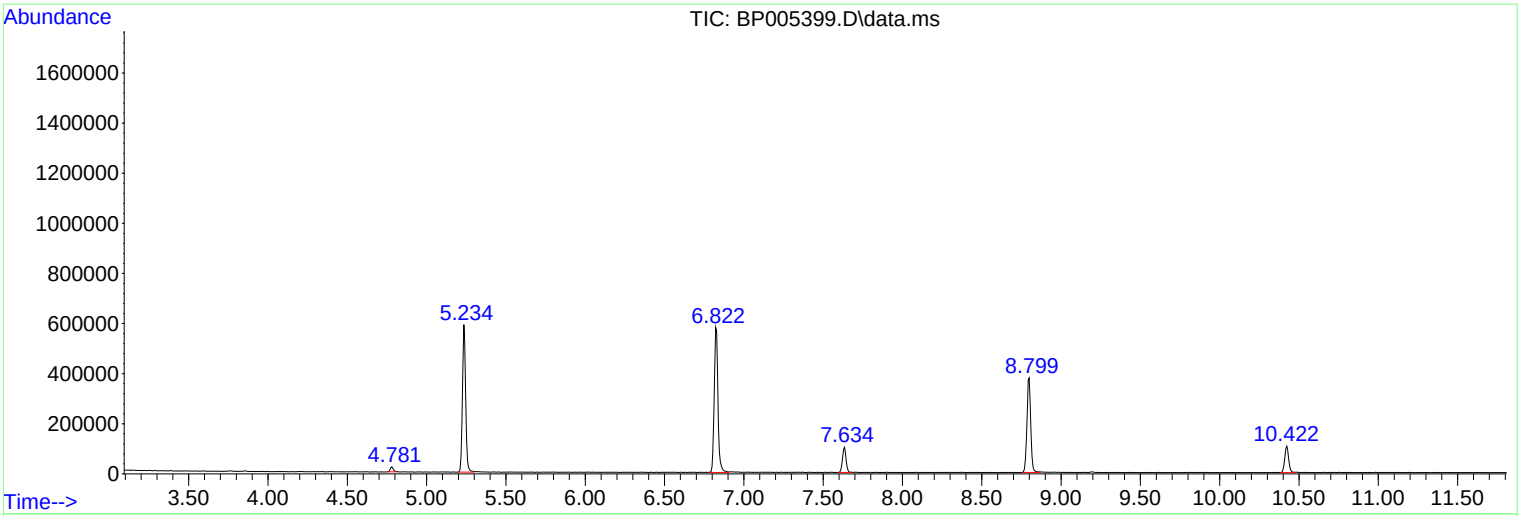
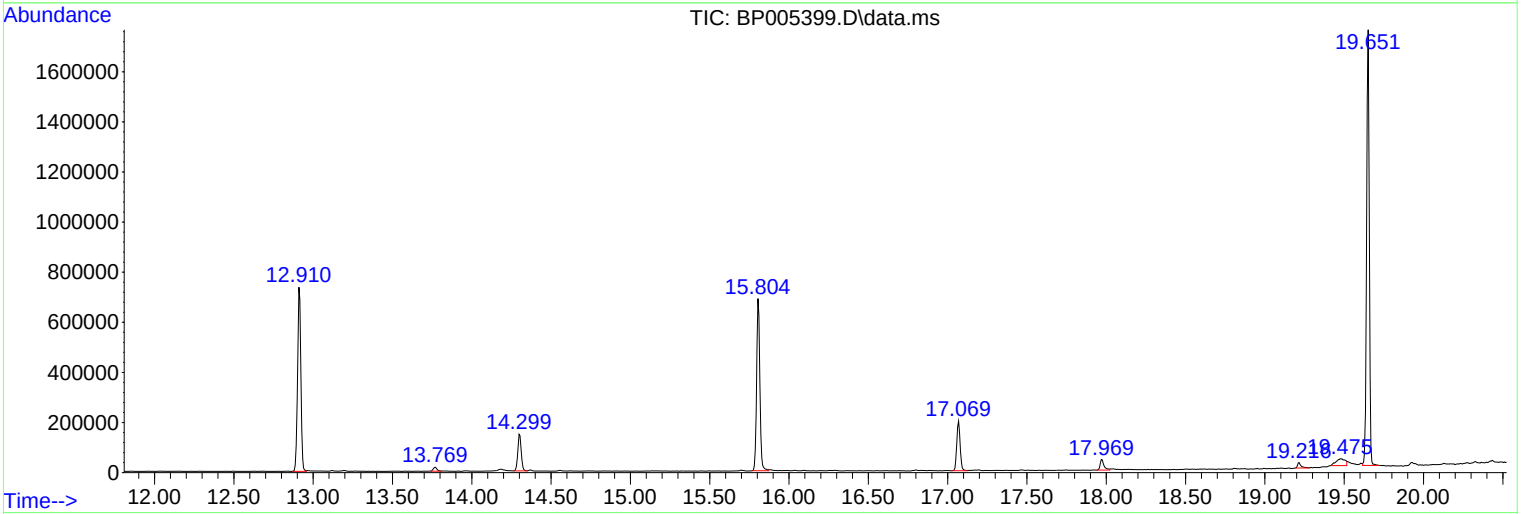
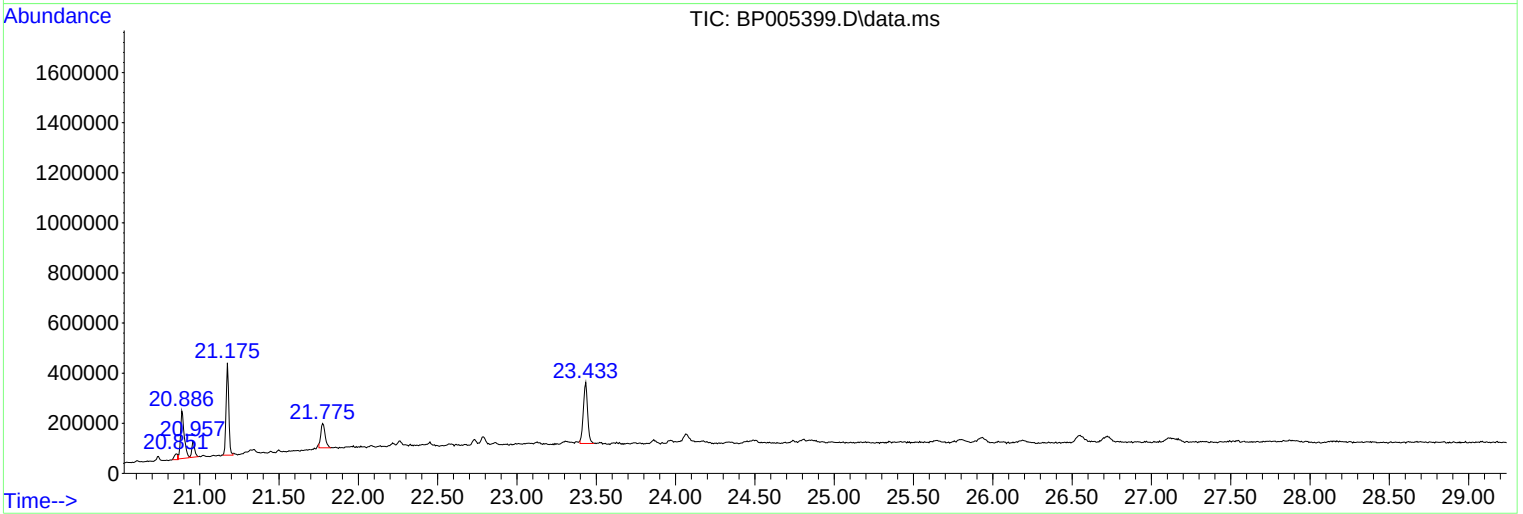
ClientSampleId :
SB-40-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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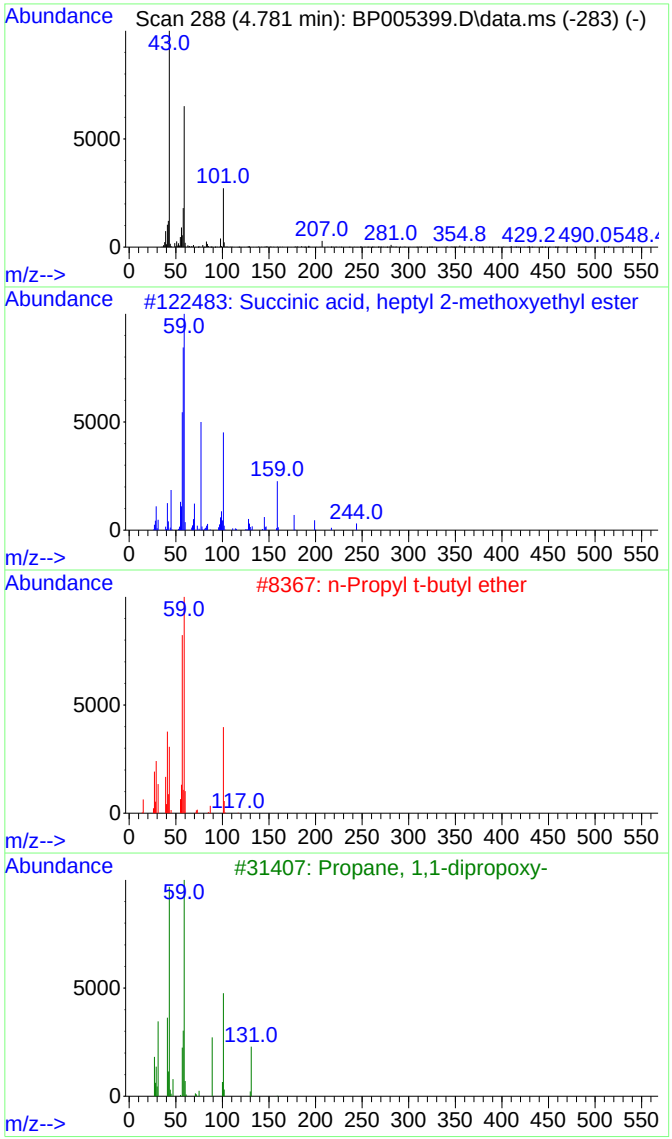
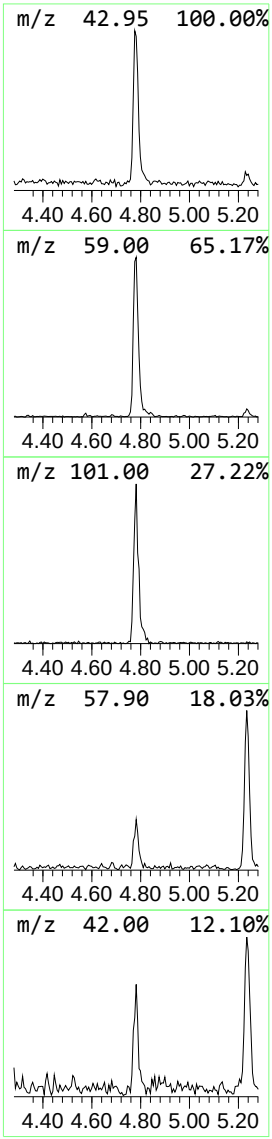
Peak Number 1 unknown4.781 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.781	3.56 ng	28098	1,4-Dichlorobenzene-d4	7.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	38
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	38
3	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	36
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5	Hexane, 1-(1-methoxyethoxy)-	160	C9H20O2	054340-90-8	23





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Misc :
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Instrument : BNA_P
ClientSampleId : SB-40-9.5-10.0

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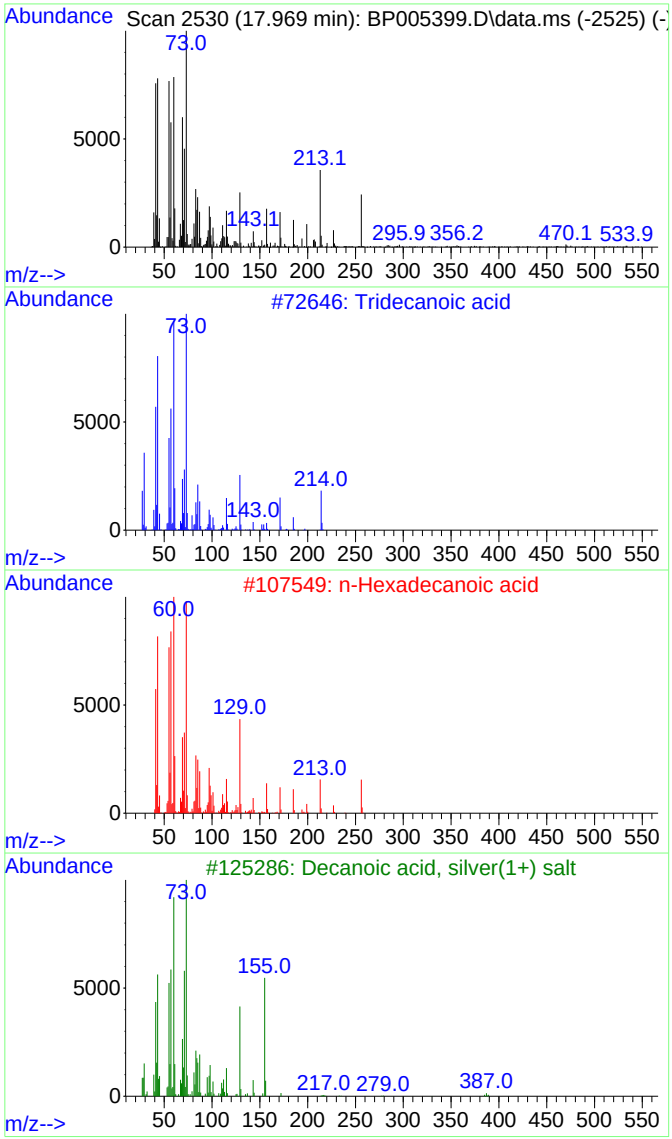
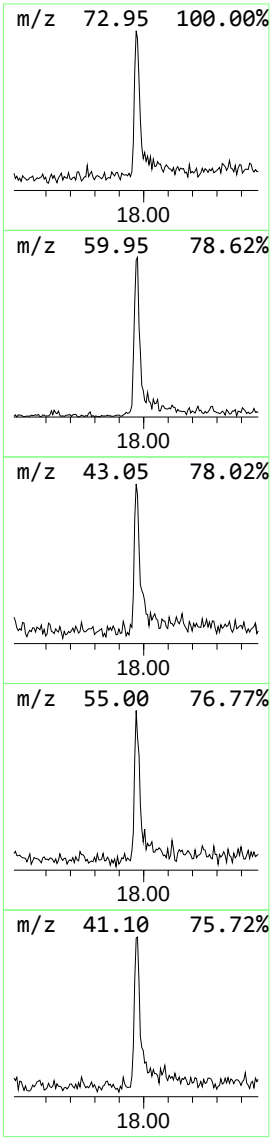
Peak Number 2 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.969	4.89 ng	70325	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





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BNA_P
ClientSampleId :
SB-40-9.5-10.0

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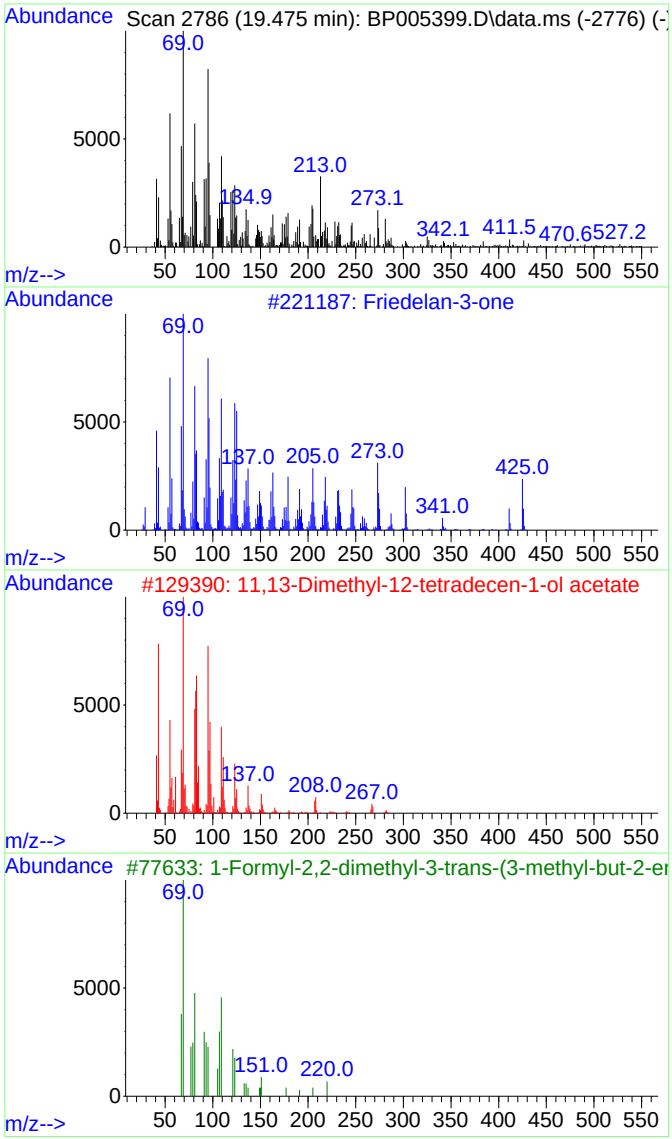
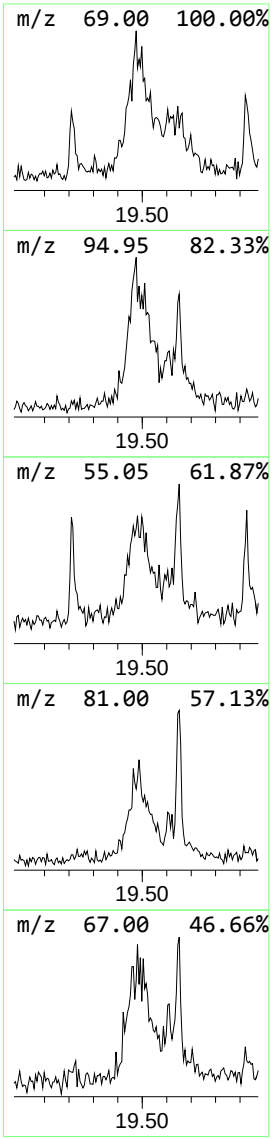
Peak Number 3 Friedelan-3-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	5.10 ng	110675	Chrysene-d12	21.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	93
2	11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	74
3	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	46
4	2-Decyne	138	C10H18	002384-70-5	43
5	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	38





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ALS Vial : 14 Sample Multiplier: 1

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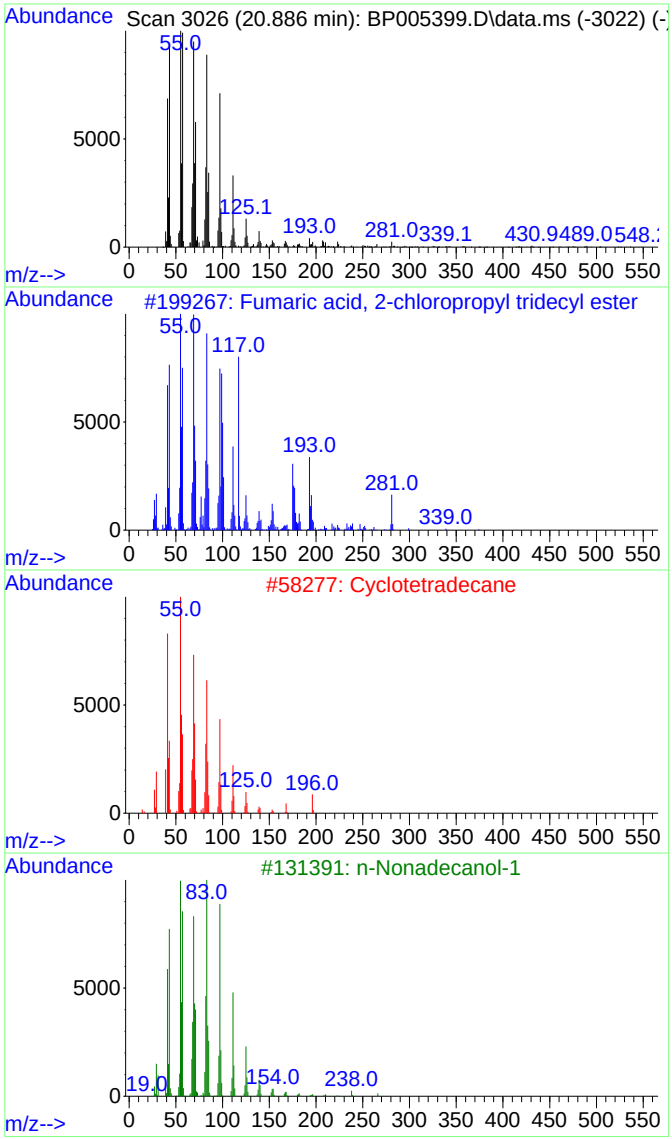
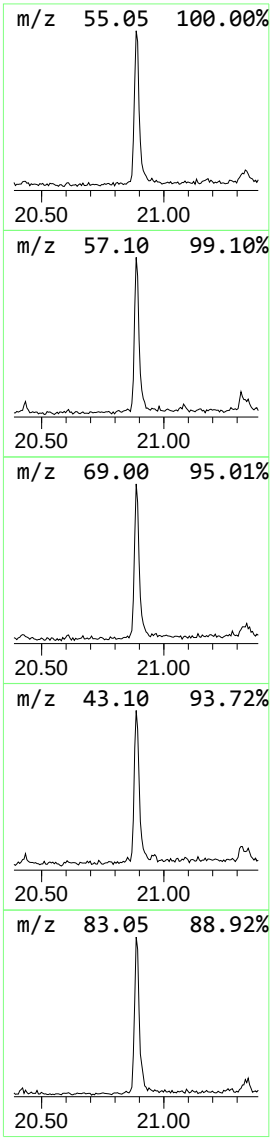
****
Peak Number 4 Fumaric acid, 2-chloropropy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	14.17 ng	307214	Chrysene-d12	21.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	97
2	Cyclotetradecane	196	C14H28	000295-17-0	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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BNA_P
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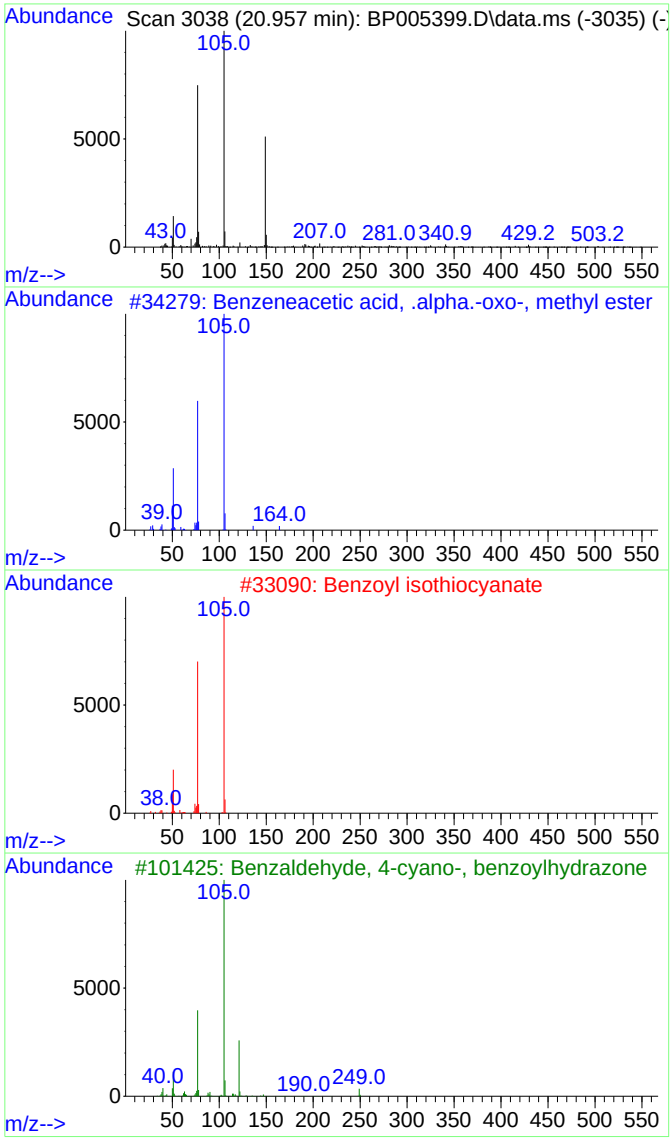
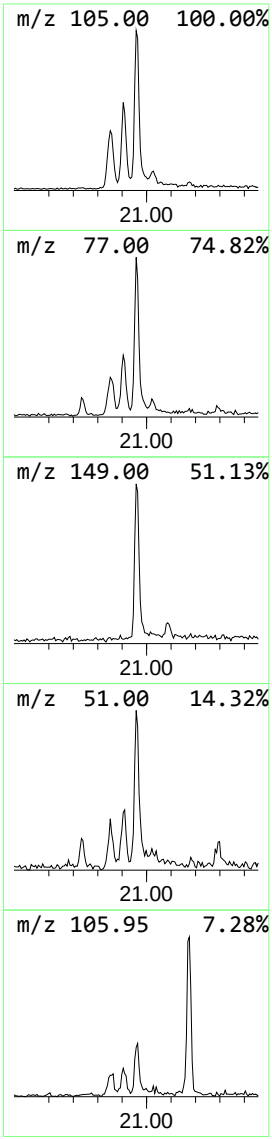
Peak Number 5 unknown20.957 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.74 ng	81185	Chrysene-d12	21.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
2	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
3	Benzaldehyde, 4-cyano-, benzoylh...	249	C15H11N3O	195066-12-7	47
4	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	47
5	2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	47





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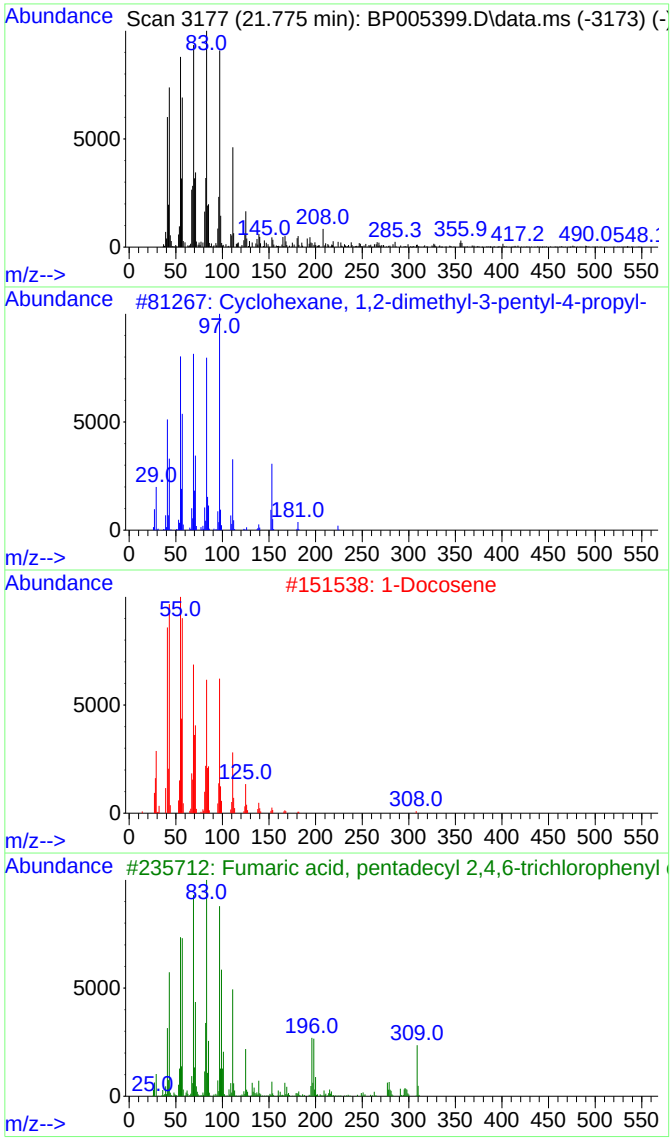
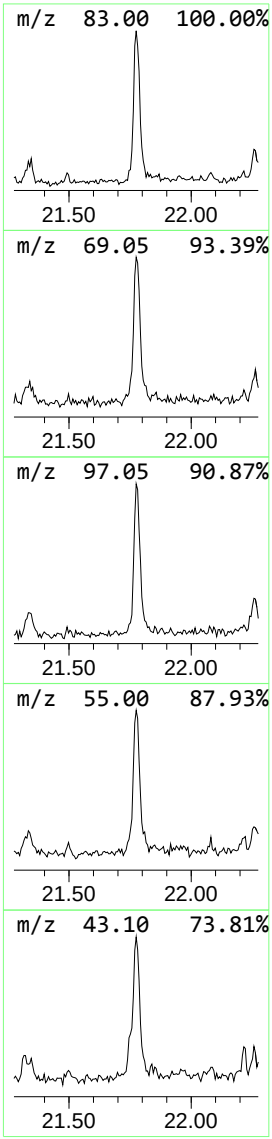
****
Peak Number 6 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.775	8.37 ng	181548	Chrysene-d12	21.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	91
2	1-Docosene	308	C22H44	001599-67-3	81
3	Fumaric acid, pentadecyl 2,4,6-t...	504	C25H35Cl3O4	1000348-27-8	80
4	Triacontyl acetate	480	C32H64O2	041755-58-2	55
5	Behenic alcohol	326	C22H46O	000661-19-8	50





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.781	4.781	3.6	ng	28098	1	7.634	157878	20.0
Tridecanoic acid	17.969	4.9	ng	70325	4	17.069	287643	20.0
Friedelan-3-one	19.475	5.1	ng	110675	5	21.175	433631	20.0
Fumaric acid, 2...	20.886	14.2	ng	307214	5	21.175	433631	20.0
unknown20.957	20.957	3.7	ng	81185	5	21.175	433631	20.0
Cyclohexane, 1,...	21.775	8.4	ng	181548	5	21.175	433631	20.0